Supporting Information

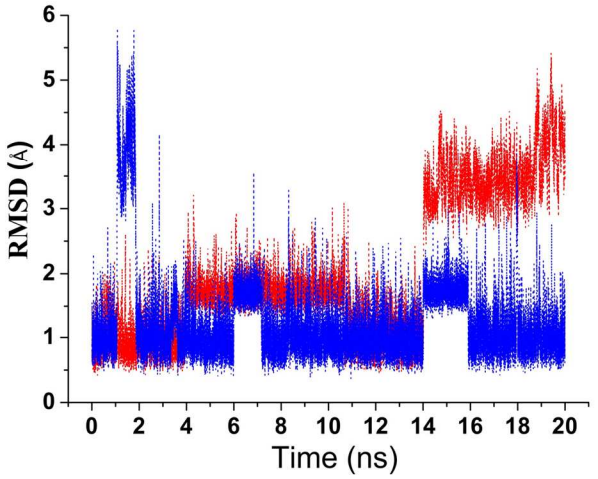
Resolution-Adapted All-Atomic and Coarse-Grained Model for Biomolecular Simulations

*Lin Shen and Hao Hu**

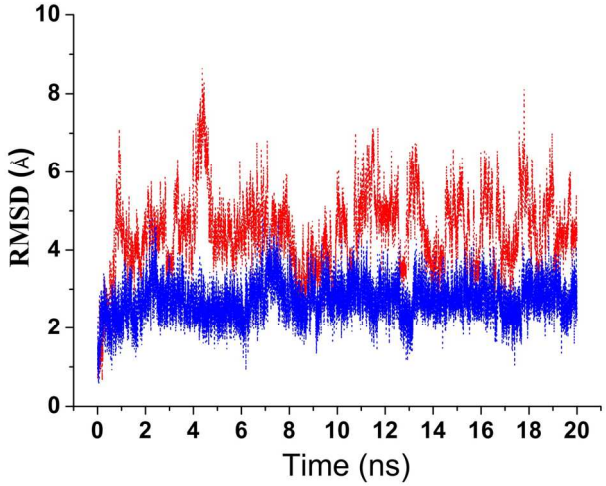
Department of Chemistry, University of Hong Kong, Pokfulam Road, Hong Kong

haohu@hku.hk

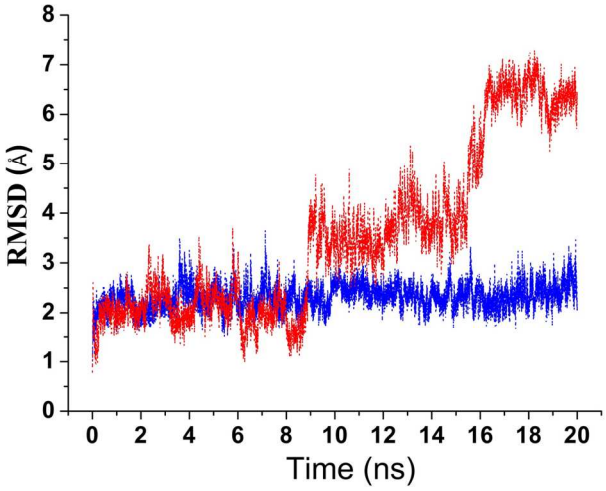
Figure S1. C_α RMSD as a function of time for one representative trajectory simulated with GB model using different cutoffs. (a) α-helix peptide 3K(I); (b) C-terminus β-hairpin of GB1; (c) ubiquitin. Different colors represent different cutoff distances: blue: 12 Å; red: 9 Å.



(a)

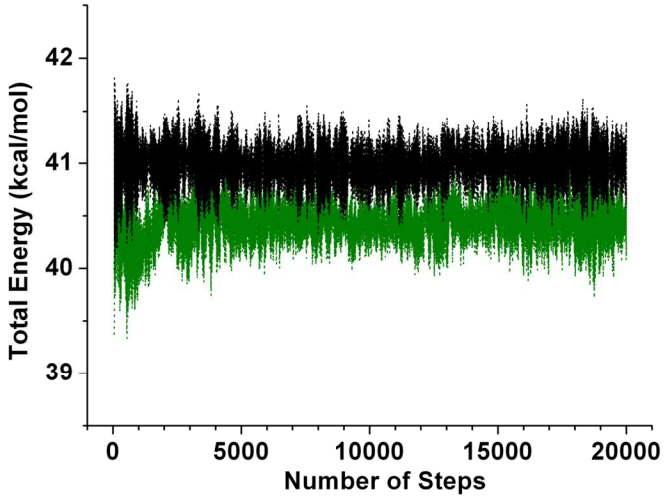


(b)

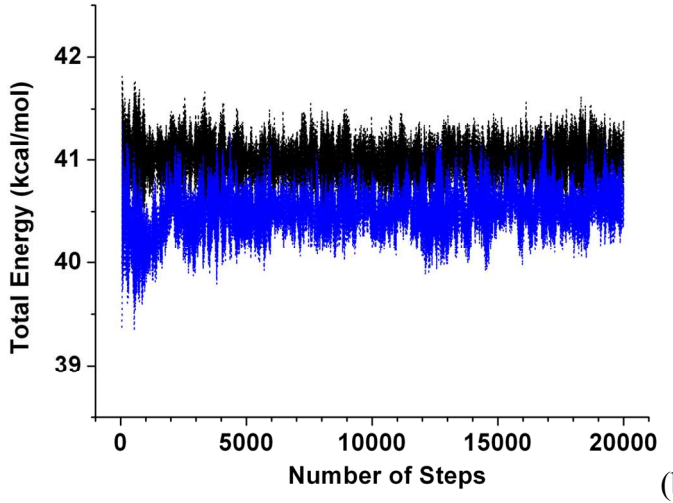


(c)

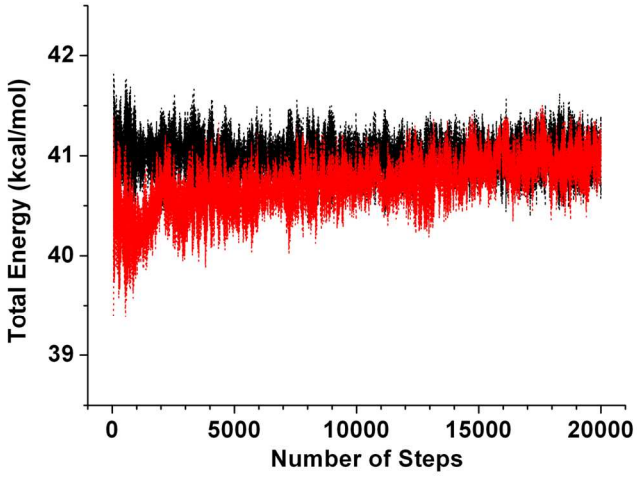
Figure S2. Total energy as a function of MD steps for one representative trajectory in the helical peptide 3K(I). Different colors represent results using different timesteps for the CG forces. Black: AA; green: AA+CG with CG timestep of 1 fs (a); blue: AA+CG with CG timestep of 10 fs (b); red: AA+CG with CG timestep of 20 fs (c).



(a)



(b)



(c)